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DUCK-TRAJECTORIES IN A THERMAL EXPLOSION PROBLEM

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Abstract—The critical values of a parameter in a thermal explosion problem in the autocatalytic case are examined by means of the method of integral manifolds and French-ducks techniques.

The system of differential equations

$$\varepsilon \frac{dx}{dt} = f(x, y, \alpha), \quad \frac{dy}{dt} = g(x, y), \tag{1}$$

where x, y are scalar variables, α is a scalar parameter, and ε is a small positive parameter, is examined. The functions f and g are supposed to be sufficiently smooth. The set of points $S = \{(x, y) : f(x, y, \alpha) = 0\}$ on the phase plane of system (1) is called the slow curve. The set of points S, where $\frac{\partial f}{\partial x} < 0$, is called the stable part of the slow curve, and the set of points S, where $\frac{\partial f}{\partial x} > 0$, is its unstable part. The trajectory of system (1) is called the duck-trajectory if it passes infinitely close to the slow curve. At first, it passes along its stable part, and then along the unstable one. In both cases, distances which are not infinitesimally small are passed [1,2].

The stable and unstable parts of the slow curve are separated by the points, at which $\frac{\partial f}{\partial x} = 0$. Such points are called irregular [3]. Usually, the investigation of system (1) in the neighbourhood of irregular points is carried out on the assumption that the inequality $\left(\frac{\partial f}{\partial x}\right)^2 + \left(\frac{\partial f}{\partial y}\right)^2 > 0$ is fulfilled at these points.

However, there is a class of problems where this condition is not fulfilled at some value of α. For example, in the system

$$\varepsilon \frac{dx}{dt} = x^2 - y^2 + \alpha, \quad \frac{dy}{dt} = 1, \tag{2}$$

with $\alpha = \pm\varepsilon$, the lines $x = \pm y$ pass along the slow curve $x^2 - y^2 + \alpha = 0$ at an infinitely long distance. Notice that the duck-trajectory is only the $x = y$ trajectory. In this example, the point $x = 0$, $y = 0$ is the point of self-intersection of the slow curve of system (2) at $\alpha = 0$. Such problems were examined in [1]. The same systems appear when considering the thermal explosion problem in the autocatalytic case. In this case, the duck-trajectories are the natural mathematical objects, which allow us modelling critical phenomena and discovering critical parameter values as asymptotic expansions involving powers of the small parameter ε. In the first-order reaction case the continuations of unstable slow integral manifolds for the calculation of the critical values of the parameter were used [4].

The system of equations of the form

$$\begin{aligned} \varepsilon \frac{d\vartheta}{d\tau} &= \eta(1-\eta)e^{\vartheta} - \alpha\,\vartheta, \\ \frac{d\eta}{d\tau} &= \eta(1-\eta)e^{\vartheta}, \end{aligned} \tag{3}$$

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in traditional dimensionless variables, is taken as a mathematical model of the thermal explosion problem in the case of an autocatalytic reaction [5]. Here, ϑ, η and τ denote the dimensionless temperature, the degree of combustion and the time, respectively, and ε is the small parameter.

In the neighbourhood of the slow curve

$$\eta(1-\eta)\,e^{\vartheta} - \alpha\,\vartheta = 0, \tag{4}$$

the system (3) has a one-dimensional slow integral manifold [6], stable at $\vartheta < 1$ and unstable at $\vartheta > 1$. At $\alpha = e/4$, the point (1,1/2) is a point of self-intersection of curve (4).

The parameter α characterizes the initial state of the system. At different values of this parameter, the reaction proceeds either into the damping regime, or into the self-accelerating regime, which leads to an explosion. The problem is to find the value of the parameter α, at which the reaction, having started in the neighbourhood of the point $\vartheta = 0$, $\eta = 0$, proceeds to the highest level of combustion of the substance given. In [4], such a value of the parameter α is called critical. The regime corresponding to this value is critical in the following sense: it is not slow, as the heating is much more than unity, and it is not explosive, as the temperature increases at the rate of the motion along the slow curve. Having determined the value of α, at which an unstable integral manifold will be a continuation of the stable integral manifold, we thus determine a critical value of α, because it is in this case that the trajectory of system (3) will move at the rate of the slow variable for the longest period of time, separating the slow and explosive regimes. Thus, the problem of finding the critical value of the parameter α becomes identical to the problem of finding such a value of α, at which the system (3) has a duck-trajectory. This value of α may be found by means of some modifications of the technique suggested in [7].

As for system (2), there are two values of parameter α

$$\alpha^* = \frac{e}{4}\left(1 - 2\sqrt{2}\,\varepsilon - \frac{49}{9}\,\varepsilon^2\right) + O\left(\varepsilon^3\right),$$
$$\alpha^{**} = \frac{e}{4}\left(1 + 2\sqrt{2}\,\varepsilon - \frac{49}{9}\,\varepsilon^2\right) + O\left(\varepsilon^3\right),$$

at which the trajectory of (3) passes along the stable and unstable parts of the slow curve (4) for times that are not infinitesimally small. The value $\alpha = \alpha^*$ corresponds to the duck-trajectory. The value $\alpha = \alpha^{**}$ is also important in the qualitative analysis of system (3). At $\alpha^{**} < \alpha$ we get a region of slow regimes and the trajectores of system (3) will pass along the stable part of the slow curve. At $\alpha < \alpha^*$ the slow curve becomes two-coupled, and the trajectory of system (3), having approached the neighbourhood of the point (1,1/2) at the rate of the slow variable, jumps into the explosive regime. The interval (α^*, α^{**}) corresponds to the transitional region.

The asymptotic expansion

$$\eta = \eta(\vartheta,\varepsilon) = v_0(\vartheta) + \varepsilon\, v_1(\vartheta) + \varepsilon^2\, v_2(\vartheta) + O\left(\varepsilon^3\right), \quad \alpha^* = \alpha_0 + \varepsilon\,\alpha_1 + \varepsilon^2\,\alpha_2 + O\left(\varepsilon^3\right),$$

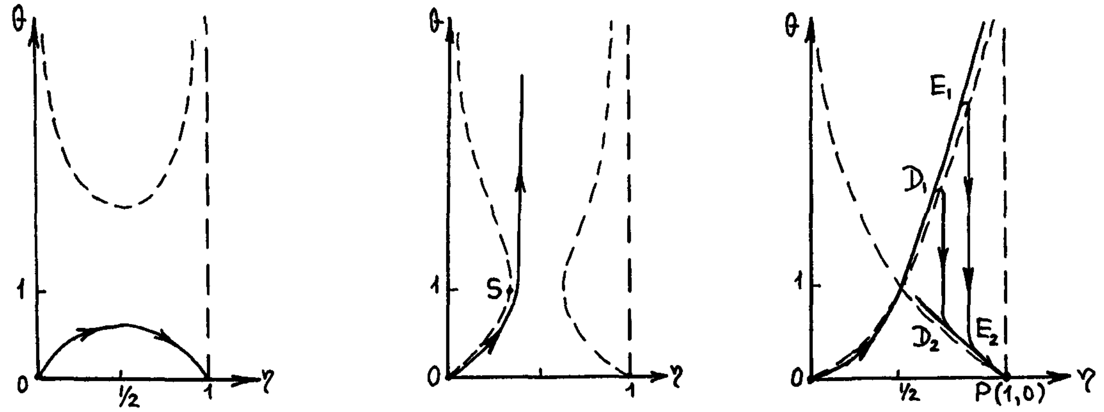
$$\alpha_0 = \frac{e}{4}, \qquad v_0 = \begin{cases} \frac{1}{2}\left(1 - \sqrt{1-\vartheta\exp(1-\vartheta)}\right), & 0 < \vartheta, < 1, \\ \frac{1}{2}\left(1 + \sqrt{1-\vartheta\exp(1-\vartheta)}\right), & \vartheta > 1, \end{cases}$$

$$\alpha_1 = -\frac{e}{\sqrt{2}}, \quad v_1 = \frac{\vartheta\left(\alpha_0 + \alpha_1 v_0'\right)}{v_0'\left(1-2v_0\right)\exp\vartheta},$$

$$\alpha_2 = -\frac{49}{36}e, \quad v_2 = \frac{\vartheta\left(\alpha_1 v_1' + \alpha_2 v_0'\right) + v_0'\, v_1^2 \exp\vartheta + v_1\left(1 - v_1'\right)\left(1-2v_0\right)}{v_0'\left(1-2v_0\right)\exp\vartheta}$$

was found for the critical duck-trajectory.

The approach suggested may be applied as well for the discovery of the critical values of the parameter in the case of an autocatalytic reaction, taking into consideration the process of thermal conductivity.



(a) The case $\alpha > e/4$—the slow regime.

(b) The case $\alpha < e/4$—the explosive regime, S is the jump point.

(c) The case $\alpha^* < \alpha' < \alpha'' < e/4$. Trajectory OE_1E_2P corresponds to the value α', trajectory OD_1D_2P—to α'', α^*—corresponds to the duck-trajectory.

Figure 1. Phase portrait of the system (3). The slow curve is shown by the broken line.

In this case, the system of equations will take the form

$$\varepsilon \frac{\partial \vartheta}{\partial \tau} = \eta(1-\eta)\, e^{\vartheta} + \frac{1}{\delta}\left(\frac{n}{\xi}\frac{\partial \vartheta}{\partial \xi} + \frac{\partial^2 \vartheta}{\partial \xi^2}\right), \tag{5}$$

$$\frac{\partial \eta}{\partial \tau} = \eta(1-\eta)\, e^{\vartheta}, \tag{6}$$

$$\vartheta(\tau, 1) = \vartheta'_{\xi}(\tau, 0) = 0, \tag{7}$$

where $\eta(0,\xi)$ and $\vartheta(0,\xi)$ are given. Here δ denotes the Frank-Kamenetskii parameter; its role is the same as that of parameter α in system (3). We put $n = 1$, limiting the study to the case of cylindrical region. Setting $\varepsilon = 0$ in (5) and using (7), we get the problem for the slow manifold $\vartheta = \vartheta_0(\eta, \xi)$

$$\vartheta_0'' + \frac{1}{\xi}\vartheta_0' + m\, e^{\vartheta_0} = 0, \qquad m = \delta\, \eta(1-\eta), \tag{8}$$

$$\vartheta_0(1) = \vartheta_0'(0) = 0. \tag{9}$$

The solution of (8), (9) is:

$$\vartheta_0 = 2\ln\frac{2\nu\kappa}{1+\xi^2\kappa^2}, \qquad \kappa = \nu \pm \sqrt{\nu^2 - 1}, \quad \nu = \sqrt{\frac{2}{m}}.$$

The condition of self-intersection of this function at the point $\eta = 1/2$, $\nu = 1$ allows us to get a zero-order approximation of the critical value of parameter $\delta = \delta(\varepsilon) : \delta(0) = 8$. Consider formal asymptotic expansions for the slow integral manifold $\vartheta = \vartheta(\eta, \xi, \varepsilon) = \vartheta_0 + \varepsilon\, \vartheta_1 + \cdots$, and for the critical value of the parameter $\delta = \delta(\varepsilon) = 8\ (1 + \varepsilon\, \delta_1 + \cdots)$ in order to calculate critical values of the parameter δ. For ϑ_1, we obtain the following boundary value problem

$$\vartheta_1'' + \frac{1}{\xi}\vartheta_1' + 8\eta(1-\eta)\, e^{\vartheta_0}\, \vartheta_1 = 8\eta(1-\eta)\, e^{\vartheta_0}\left(\frac{\partial \vartheta_0}{\partial \eta} - \delta_1\right),$$

$$\vartheta_1(1) = \vartheta_1'(0) = 0.$$

The eigenfunction of the corresponding homogeneous boundary value problem has the form $\vartheta = (1-\xi^2)/(1+\xi^2)$. The condition of existence of the solution of the nonhomogeneous boundary value problem for ϑ_1 has the form:

$$\int_0^1 \left(\frac{\partial \vartheta_0}{\partial \eta} - \delta_1\right) \frac{1-\xi^2}{(1+\xi^2)^3}\, d\xi = 0, \qquad \frac{\partial \vartheta_0}{\partial \eta} = \pm 4 \frac{1-\xi^2}{1+\xi^2}.$$

From the last equation, we obtain

$$\delta^* = 8\left(1 + \varepsilon \frac{4}{3} \frac{8+3\pi}{4+\pi}\right) + O\left(\varepsilon^2\right),$$
$$\delta^{**} = 8\left(1 - \varepsilon \frac{4}{3} \frac{8+3\pi}{4+\pi}\right) + O\left(\varepsilon^2\right).$$

The value δ^* corresponds to the duck-trajectory, and is the critical value of δ. The interval (δ^{**}, δ^*) corresponds to the transitional regimes.

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